

Fig. 1

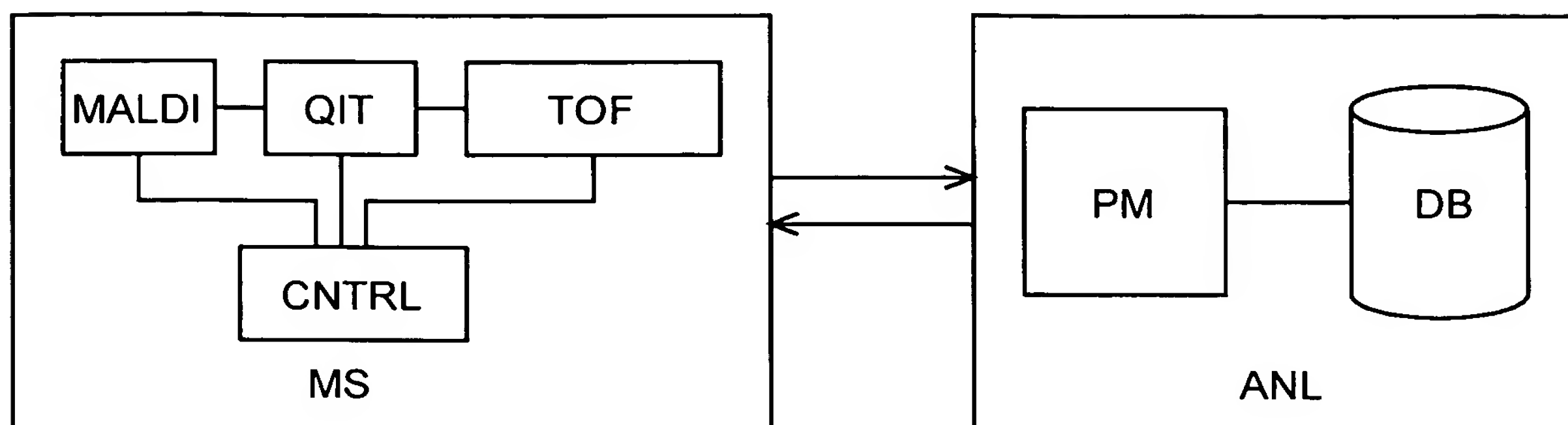


Fig. 2

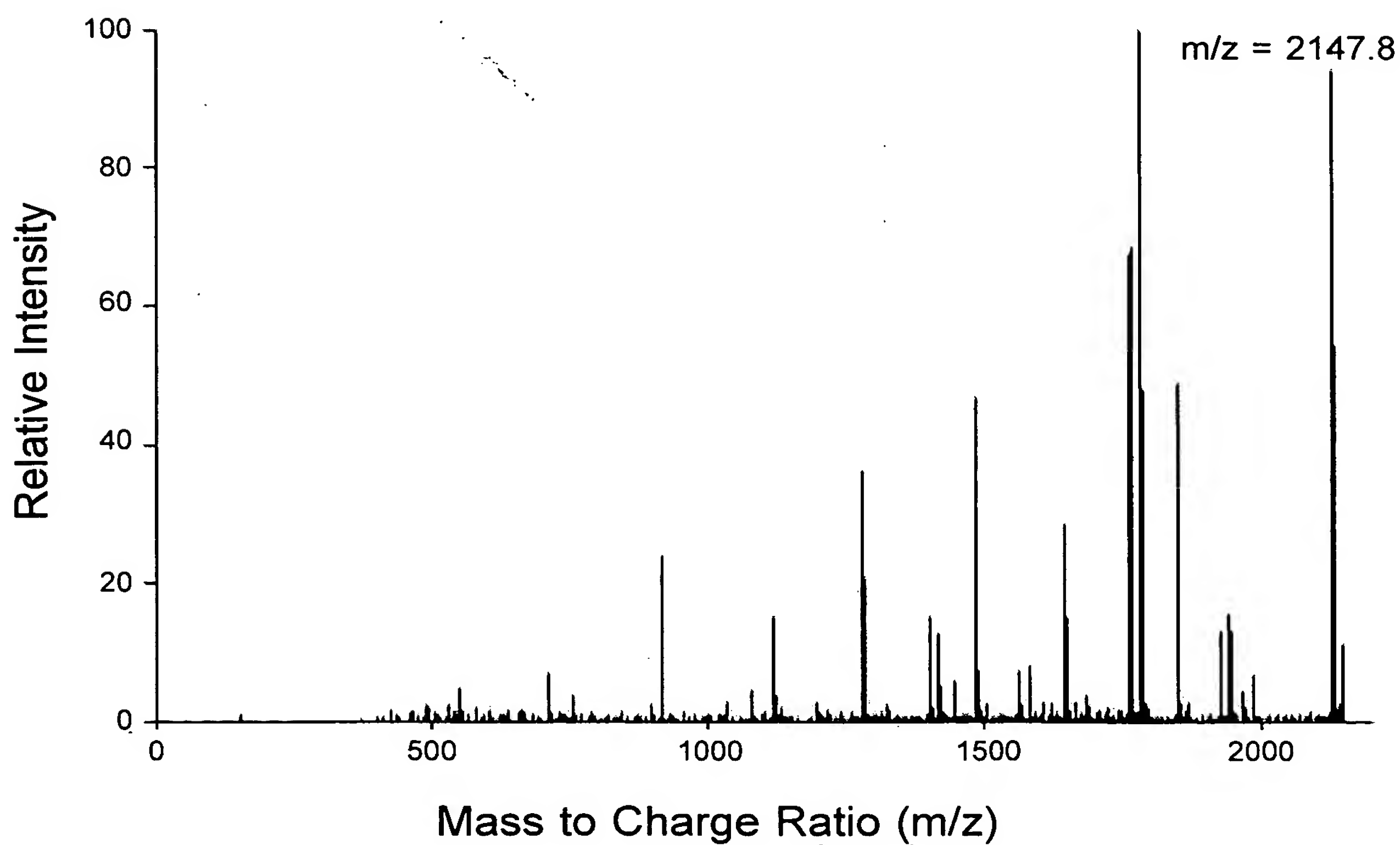
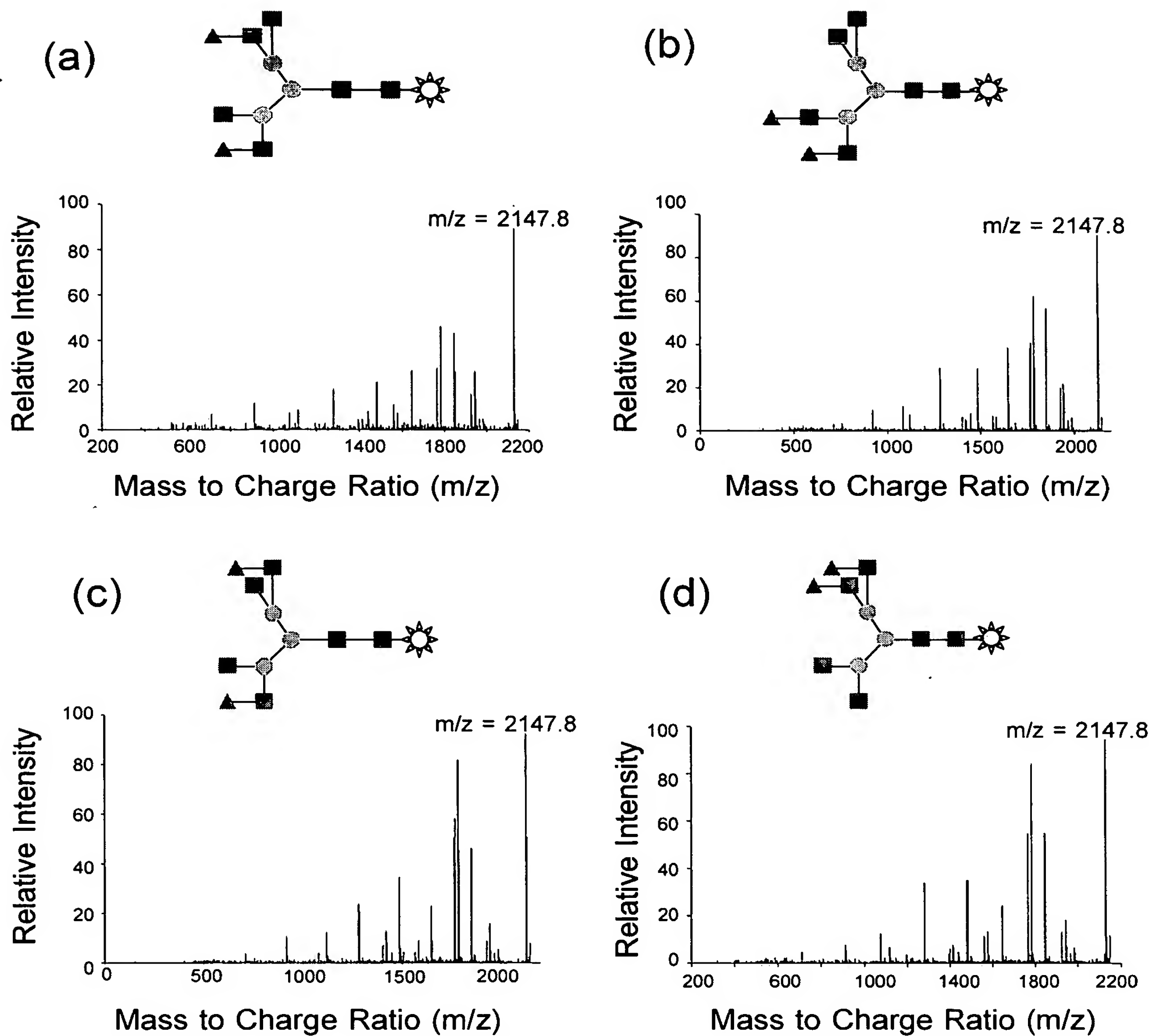
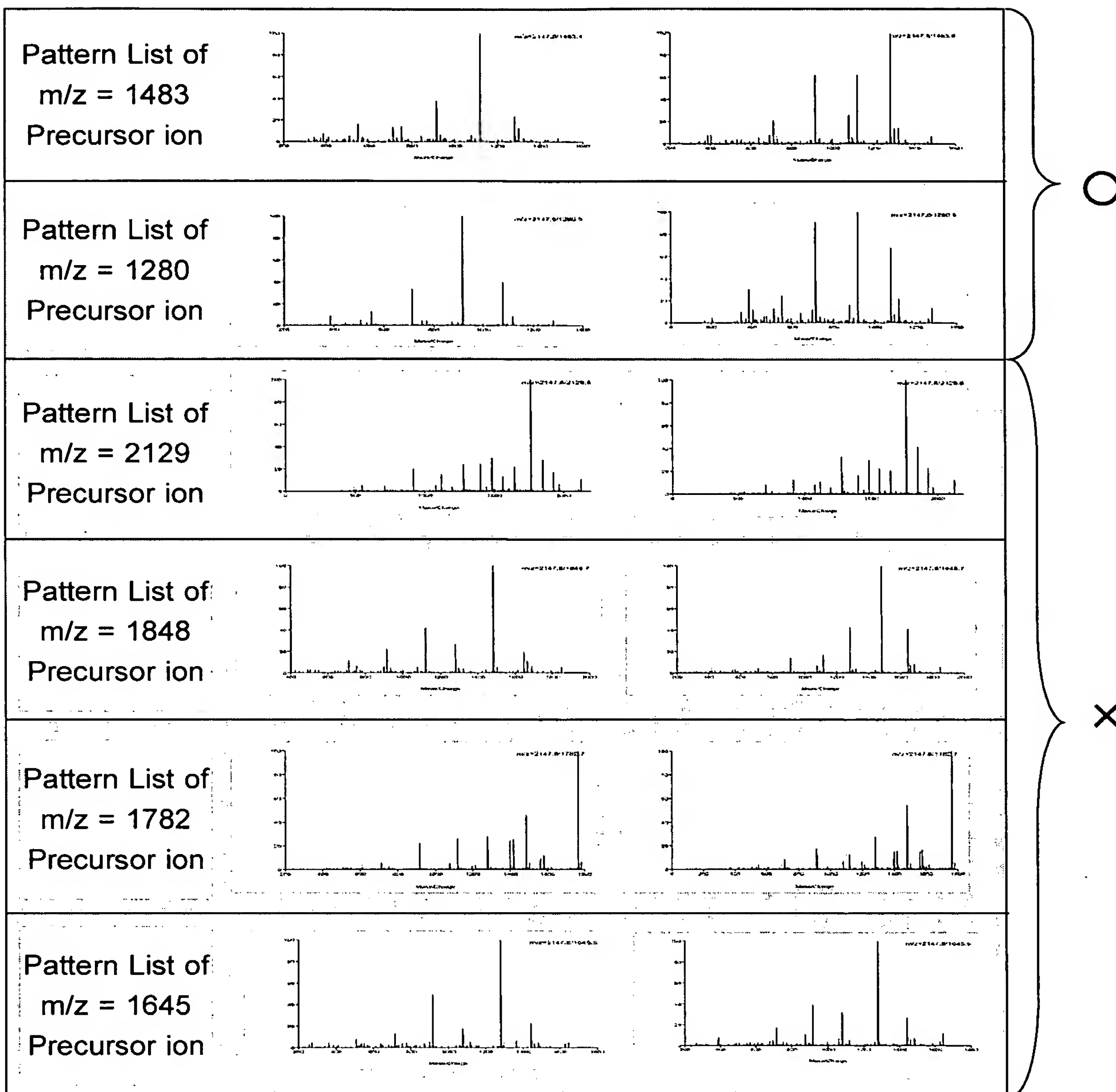


Fig. 3



| Fragment Pattern | Similarity Index<br>$S((1/D) * 1E+7)$ |          |
|------------------|---------------------------------------|----------|
|                  | S1                                    | S2       |
| (a)              | 655.813                               | 657.606  |
| (b)              | 1535.890                              | 1539.660 |
| (c)              | 4570.276                              | 4623.254 |
| (d)              | 3717.617                              | 3768.091 |

Fig. 4



| Precursor Ion | Similarity Index<br>$S((1/D) * 1E+7)$ |          | Order |
|---------------|---------------------------------------|----------|-------|
|               | S1                                    | S2       |       |
| m/z=1483      | 1165.564                              | 1149.987 | 2     |
| m/z=1280      | 1140.334                              | 1126.347 | 1     |
| m/z=2129      | 9159.474                              | 9079.574 | -     |
| m/z=1848      | 3039.331                              | 2810.509 | -     |
| m/z=1782      | 7898.673                              | 8011.952 | -     |
| m/z=1645      | 2881.634                              | 2714.678 | -     |

Fig. 5

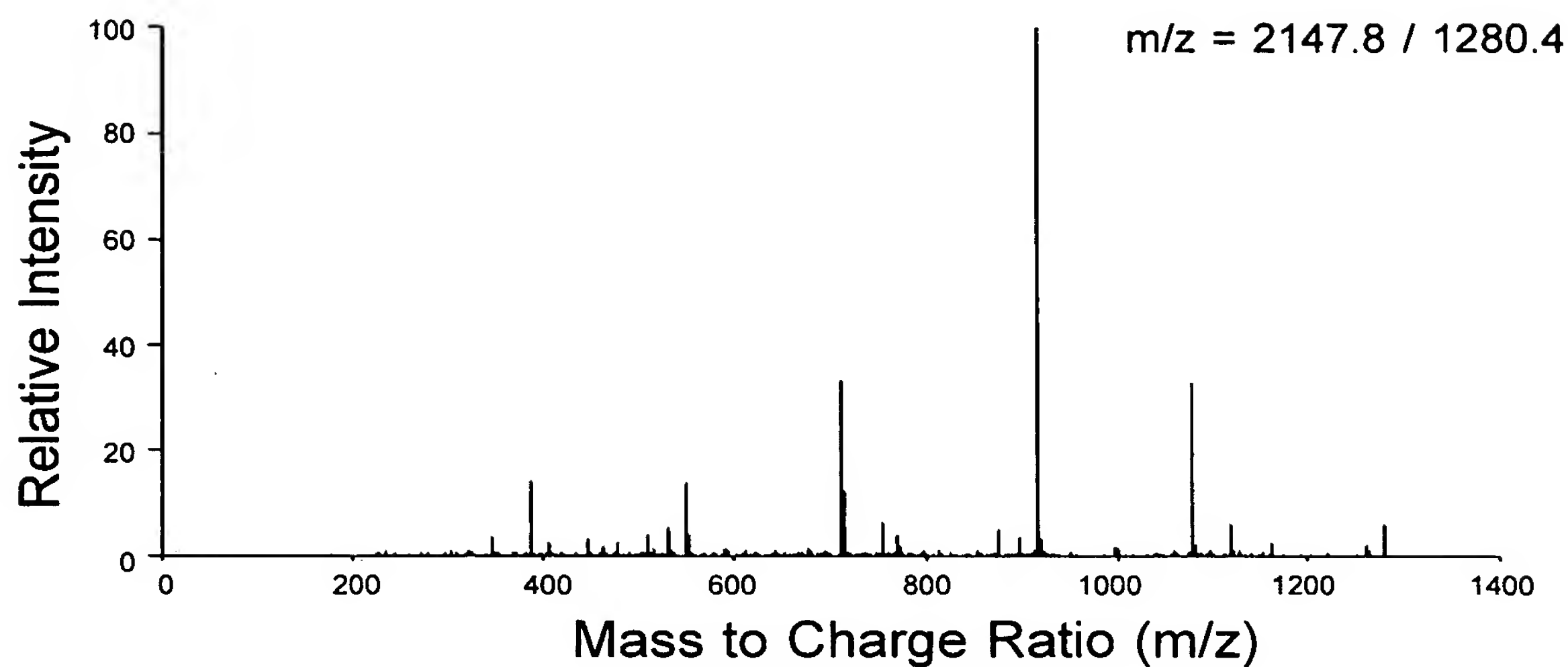
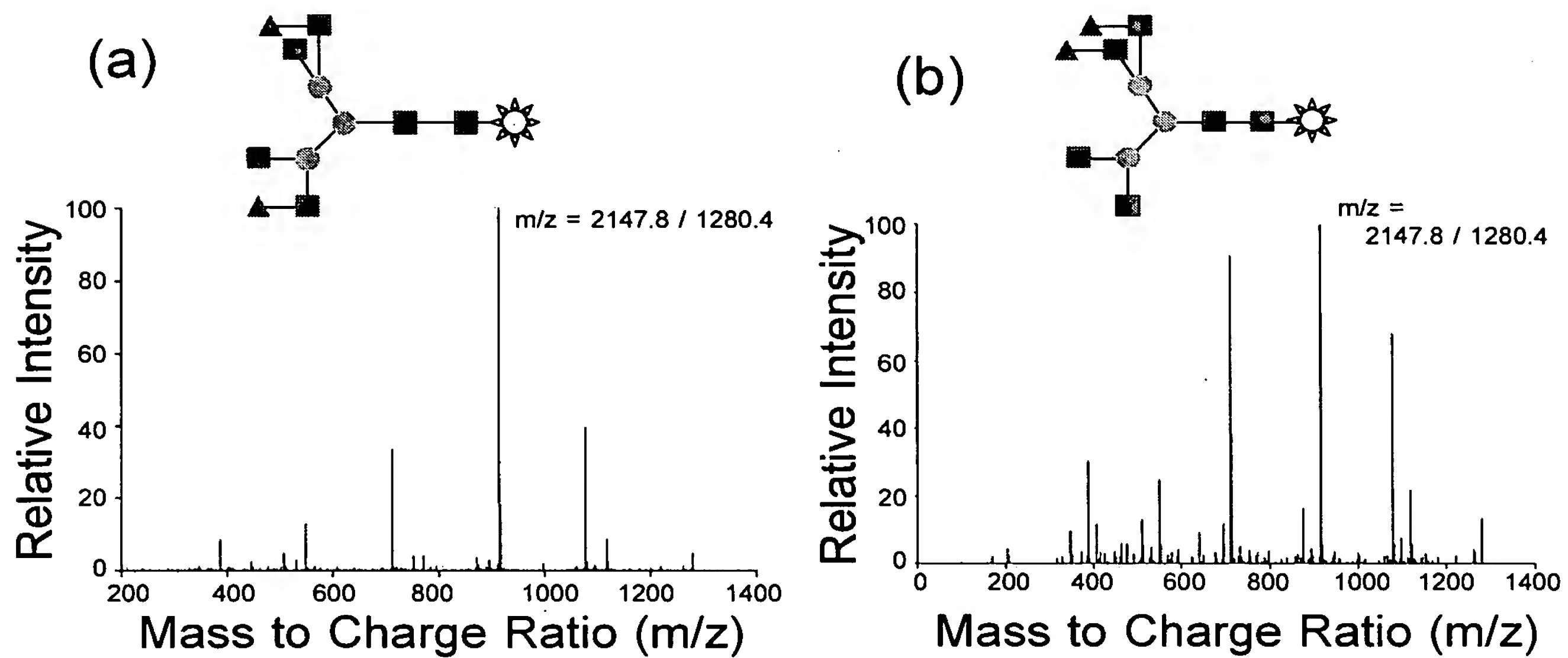
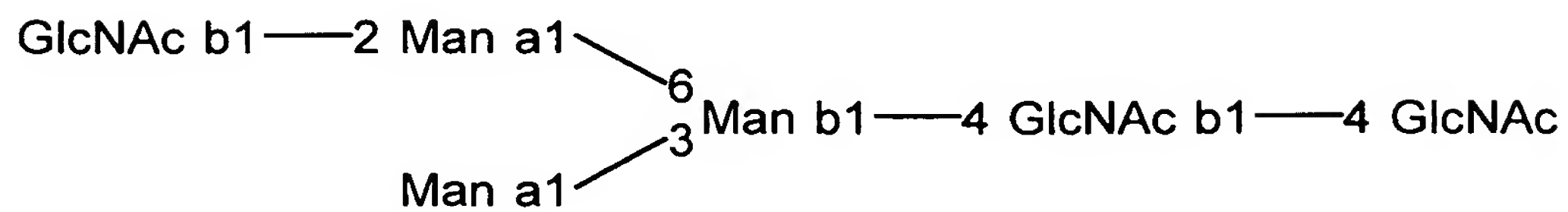


Fig. 6

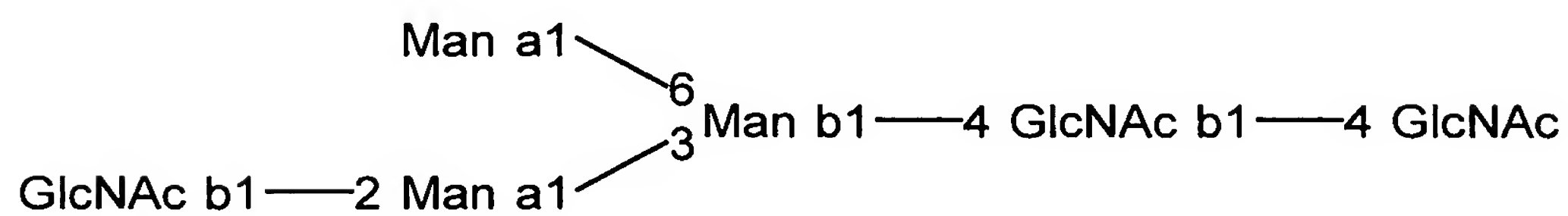


| Fragment Pattern | Similarity Index<br>$S((1/D) * 1E+7)$ |           |   |
|------------------|---------------------------------------|-----------|---|
|                  | S1                                    | S2        |   |
| (a)              | 45166.527                             | 45592.317 | ○ |
| (b)              | 1158.701                              | 1138.003  | × |

Fig. 7



(a) ONA—00001a(100.1)



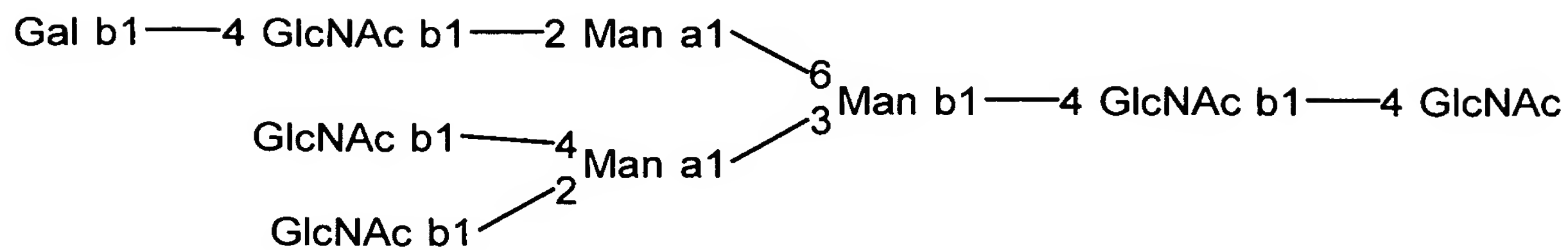
(b) ONA—00001b(100.2)

Fig. 8

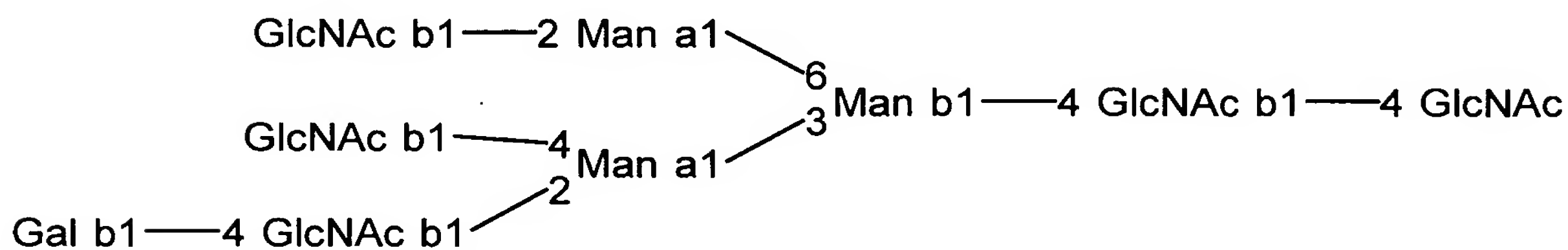
| Measured Sample   | pre-cursor ion | MS <sup>n</sup> | Dissimilarity between Same Samples |             | Peak List of Lowest Dissimilarity among Different Structures | Dissimilarity between Isomers |          |
|-------------------|----------------|-----------------|------------------------------------|-------------|--|-------------------------------|----------|
| ONA-00001a(100.1) | 1214           | 2               | 102.8163667                        | 102.8163667 | 100.2PA-MS2-1214-1.txt                                       | 100.8827                      | 100.9693 |
| ONA-00001a(100.1) | 915            | 3               | 156.28585                          | 156.28585   | 100.2PA-MS3-915-1.txt  | 287.2622                      | 297.0102 |
| ONA-00001a(100.1) | 1196           | 3               | 218.16315                          | 218.16315   | 100.2PA-MS3-1196-1.txt                                       | 424.273                       | 433.6466 |
| ONA-00001b(100.2) | 1214           | 2               | 87.27248333                        | 87.27248333 | 100.1PA-MS2-1214-3.txt                                       | 100.319                       | 100.8947 |
| ONA-00001b(100.2) | 915            | 3               | 297.8943833                        | 297.8943833 | 100.1PA-MS3-915-3.txt  | 297.0102                      | 287.2622 |
| ONA-00001b(100.2) | 1196           | 3               | 133.9454                           | 133.9454    | 100.1PA-MS3-1196-1.txt                                       | 433.6466                      | 424.273  |



Fig. 11



(e) ONG—00001e(310.2)

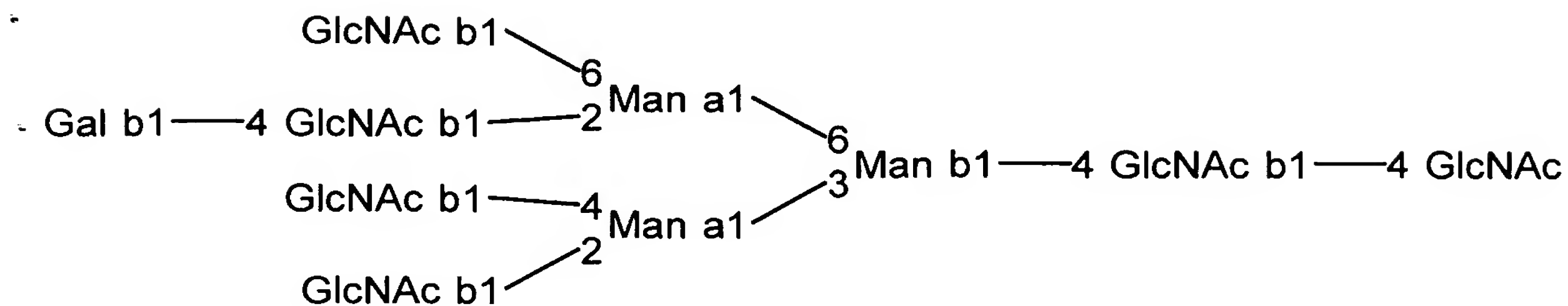


(f) ONG—00001f(310.3)

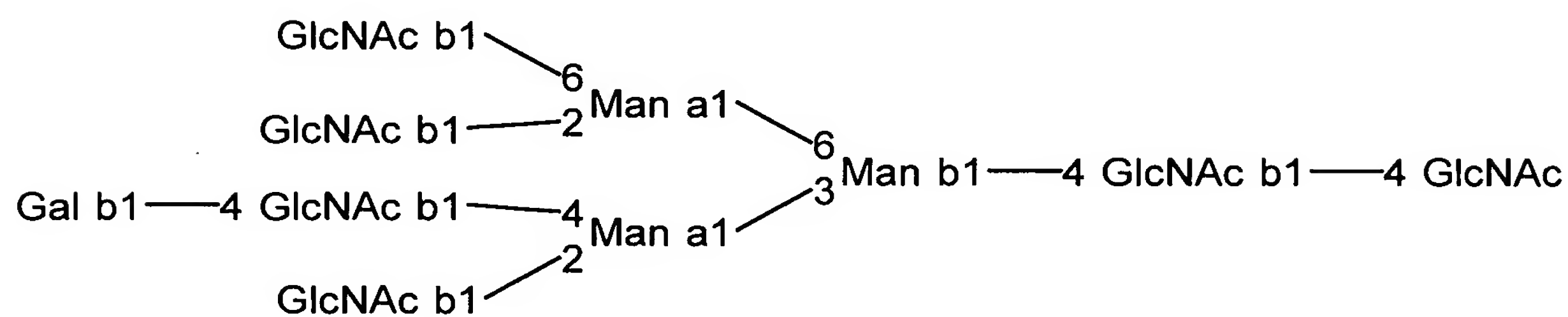
Fig. 12

| Measured Sample   | pre-cursor ion | MS <sup>n</sup> | Dissimilarity between Same Samples |             | Peak List of Lowest Dissimilarity among Different Structures | Dissimilarity between Isomers |           |
|-------------------|----------------|-----------------|------------------------------------|-------------|--|-------------------------------|-----------|
| ONG-00001e(310.2) | 1928           | 2               | 312.2041667                        | 312.2041667 | 310.3PA-MS2-1928-1.txt                                       | 160.0158                      | 155.7346  |
| ONG-00001e(310.2) | 1280           | 3               | 655.3959833                        | 655.3959833 | 310.3PA-MS3-1280-1.txt                                       | 1596.9166                     | 1523.2752 |
| ONG-00001e(310.2) | 1483           | 3               | 174.4776167                        | 174.4776167 | 310.3PA-MS3-1483-2.txt                                       | 119.2134                      | 114.7385  |
| ONG-00001f(310.3) | 1928           | 2               | 205.0538167                        | 205.0538167 | 310.2PA-MS2-1928-3.txt                                       | 155.7346                      | 160.0158  |
| ONG-00001f(310.3) | 1280           | 3               | 290.52645                          | 290.52645   | 100.2PA-MS3-1196-2.txt                                       | 1116.8702                     | 1120.5336 |
| ONG-00001f(310.3) | 1483           | 3               | 327.5316067                        | 327.5316067 | 310.2PA-MS3-1483-2.txt                                       | 114.7385                      | 119.2134  |

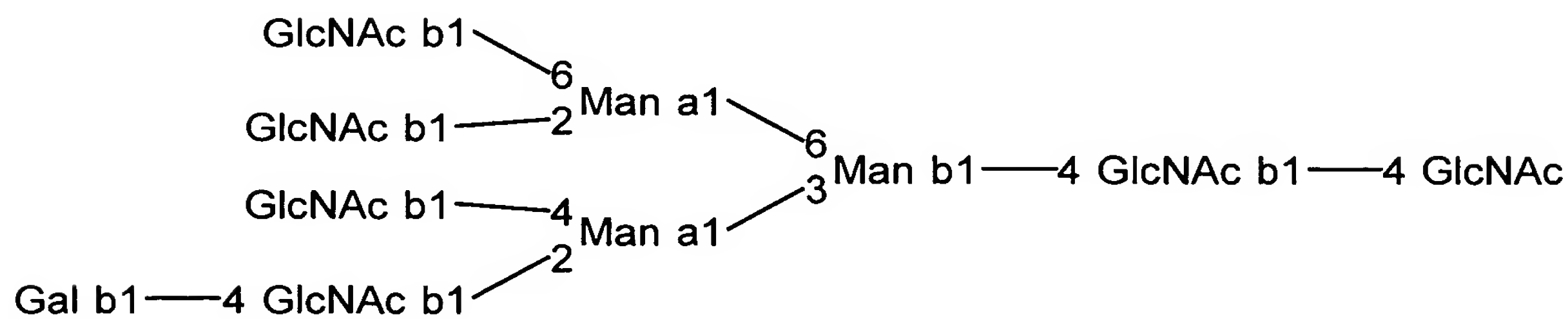
Fig. 13



(a) ONG—000020(400.2)



(b) ONG—000021(400.3)



(c) ONG—000022(400.5)



Fig. 14

| Measured Sample   | pre-cursor ion | MS <sup>n</sup> | Dissimilarity between Same Samples |             | Peak List of Lowest Dissimilarity among Different Structures | Dissimilarity between Isomers |           |
|-------------------|----------------|-----------------|------------------------------------|-------------|--|-------------------------------|-----------|
| ONG-000020(400.2) | 1985           | 2               | 858.4422167                        | 858.4422167 | 400.5PA-MS2-1985-2.txt                                       | 1864.9315                     | 1859.783  |
| ONG-000020(400.2) | 1321           | 3               | 91.71695                           | 91.71695    | 400.3PA-MS3-1321-3.txt                                       | 78.5283                       | 72.082    |
| ONG-000020(400.2) | 1483           | 3               | 411.9361833                        | 411.9361833 | 400.5PA-MS3-1483-3.txt                                       | 239.7108                      | 267.7883  |
| ONG-000020(400.2) | 1602           | 3               | 969.9182                           | 969.9182    | 400.5PA-MS3-1602-3.txt                                       | 1103.5193                     | 1101.6843 |
| ONG-000020(400.2) | 1686           | 3               | 533.01535                          | 533.01535   | 400.5PA-MS3-1686-2.txt                                       | 3936.2343                     | 3955.8892 |
| ONG-000020(400.2) | 1764           | 3               | 378.8141                           | 378.8141    | 400.5PA-MS3-1764-2.txt                                       | 4367.2301                     | 4411.4233 |
| ONG-000020(400.2) | 1967           | 3               | 281.67725                          | 281.67725   | No Spectrum under 10000                                      |                               |           |
| ONG-000021(400.3) | 1985           | 2               | 455.7612167                        | 455.7612167 | 400.5PA-MS2-1985-1.txt                                       | 257.98                        | 250.1656  |
| ONG-000021(400.3) | 1321           | 3               | 123.00805                          | 123.00805   | 400.5PA-MS3-1321-1.txt                                       | 42.8943                       | 45.8055   |
| ONG-000021(400.3) | 1483           | 3               | 256.8724167                        | 256.8724167 | 310.2PA-MS3-1483-3.txt                                       | 1801.5073                     | 1739.7947 |
| ONG-000021(400.3) | 1602           | 3               | 338.1913972                        | 338.1913972 | 400.5PA-MS3-1602-1.txt                                       | 353.2306                      | 352.4087  |
| ONG-000021(400.3) | 1686           | 3               | 307.1847167                        | 307.1847167 | 400.5PA-MS3-1686-3.txt                                       | 3834.4255                     | 3836.0349 |
| ONG-000021(400.3) | 1764           | 3               | 813.7935                           | 813.7935    | 400.5PA-MS3-1764-1.txt                                       | 5369.3515                     | 5352.7886 |
| ONG-000021(400.3) | 1967           | 3               | 800.1308                           | 800.1308    | 400.5PA-MS3-1967-2.txt                                       | 6323.3696                     | 6343.6005 |
| ONG-000022(400.5) | 1985           | 2               | 283.9350667                        | 283.9350667 | 400.3PA-MS2-1985-2.txt                                       | 250.1656                      | 257.98    |
| ONG-000022(400.5) | 1321           | 3               | 106.6899667                        | 106.6899667 | 400.3PA-MS3-1321-2.txt                                       | 45.8055                       | 42.8943   |
| ONG-000022(400.5) | 1483           | 3               | 256.8044                           | 256.8044    | 400.2PA-MS3-1483-3.txt                                       | 267.7883                      | 239.7108  |
| ONG-000022(400.5) | 1602           | 3               | 700.73915                          | 700.73915   | 400.3PA-MS3-1602-3.txt                                       | 352.4087                      | 353.2306  |
| ONG-000022(400.5) | 1686           | 3               | 720.2411167                        | 720.2411167 | 400.3PA-MS3-1686-1.txt                                       | 3836.0349                     | 3834.4255 |
| ONG-000022(400.5) | 1764           | 3               | 1014.059233                        | 1014.059233 | 400.2PA-MS3-1764-2.txt                                       | 4411.4233                     | 4367.2301 |
| ONG-000022(400.5) | 1967           | 3               | 513.7448222                        | 513.7448222 | 400.3PA-MS3-1967-3.txt                                       | 6343.6005                     | 6323.3696 |

Fig. 15

